

Supplementary Materials: iPPBS–Opt: A Sequence–Based Ensemble Classifier for Identifying Protein–Protein Binding Sites by Optimizing Imbalanced Training Dataset

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Table S1. Dataset. List of the 99 proteins and their residues' attributions associated with the protein–protein binding sites. (1) Those labeled with 1 and 0 in column 4 are of surface and non–surface residues, respectively; (2) Those labeled with 1 and –1 in column 5 are of interface and non–interface residues, respectively.

Protein ID	Chain ID	Residue Position	Surface	Interface
1ACB	E	1	1	–1
1ACB	E	2	0	–1
1ACB	E	3	1	–1
1ACB	E	4	0	–1
1ACB	E	5	1	–1
1ACB	E	6	0	–1
1ACB	E	7	1	–1
1ACB	E	8	0	–1
1ACB	E	9	1	–1
1ACB	E	10	0	–1
1ACB	E	11	1	–1
1ACB	E	12	1	–1
1ACB	E	13	1	–1
1ACB	E	16	0	–1
1ACB	E	17	0	–1
1ACB	E	18	1	–1
1ACB	E	19	1	–1
1ACB	E	20	1	–1
1ACB	E	21	1	–1
1ACB	E	22	0	–1
1ACB	E	23	1	–1
1ACB	E	24	1	–1
1ACB	E	25	0	–1
1ACB	E	26	0	–1
1ACB	E	27	0	–1
1ACB	E	28	0	–1
1ACB	E	29	0	–1
1ACB	E	30	0	–1
1ACB	E	31	0	–1
1ACB	E	32	0	–1
1ACB	E	33	0	–1
1ACB	E	34	0	–1
1ACB	E	35	1	–1
1ACB	E	36	1	–1
1ACB	E	37	1	–1
1ACB	E	38	1	–1
1ACB	E	39	1	1
1ACB	E	40	0	–1

1ACB	E	41	1	1
1ACB	E	42	0	-1
1ACB	E	43	0	-1
1ACB	E	44	0	-1
1ACB	E	45	0	-1
1ACB	E	46	0	-1
1ACB	E	47	0	-1
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1ACB	E	59	1	1
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1ACB	E	61	1	-1
1ACB	E	62	1	-1
1ACB	E	63	1	-1
1ACB	E	64	0	-1
1ACB	E	65	0	-1
1ACB	E	66	0	-1
1ACB	E	67	0	-1
1ACB	E	68	0	-1
1ACB	E	69	0	-1
1ACB	E	70	0	-1
1ACB	E	71	0	-1
1ACB	E	72	0	-1
1ACB	E	73	1	-1
1ACB	E	74	1	-1
1ACB	E	75	1	-1
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1ACB	E	77	1	-1
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1ACB	E	91	0	-1
1ACB	E	92	1	-1

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1ACB	E	95	1	-1
1ACB	E	96	1	-1
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1ACB	E	144	1	-1

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1ACB	E	196	0	-1
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1ACB	E	198	0	-1

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1AGR	A	9	1	-1
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1AGR	A	255	1	-1
1AGR	A	256	1	-1
1AGR	A	257	1	-1

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1AGR	A	260	1	-1
1AGR	A	261	0	-1
1AGR	A	262	0	-1
1AGR	A	263	0	-1
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1AGR	A	266	0	-1
1AGR	A	267	0	-1
1AGR	A	268	0	-1
1AGR	A	269	0	-1
1AGR	A	270	0	-1
1AGR	A	271	1	-1
1AGR	A	272	0	-1
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1DVF	D	101	1	1

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1QFU	A	274	1	1
1QFU	A	275	1	-1
1QFU	A	276	1	1
1QFU	A	277	1	-1
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1QFU	A	281	0	-1
1QFU	A	282	0	-1
1QFU	A	283	0	-1
1QFU	A	284	0	-1
1QFU	A	285	1	-1

1QFU	A	286	0	-1
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1QFU	A	288	0	-1
1QFU	A	289	1	-1
1QFU	A	290	1	1
1QFU	A	291	1	1
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1QFU	B	10	0	-1
1QFU	B	11	1	1
1QFU	B	12	1	1

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1QFU	B	15	1	1
1QFU	B	16	1	1
1QFU	B	17	0	-1
1QFU	B	18	1	-1
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1QFU	B	166	0	-1
1QFU	B	167	1	-1
1QFU	B	168	1	-1

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1QFU	B	172	1	-1
1QFU	B	173	1	-1
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1QFU	L	134	0	-1
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1QFU	L	136	0	-1

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1QFU	L	142	1	1
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